

(FILE 'HOME' ENTERED AT 10:43:51 ON 13 SEP 2006)

FILE 'REGISTRY' ENTERED AT 10:44:01 ON 13 SEP 2006

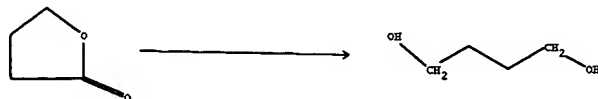
L1 1 S 1,4-BUTANEDIOL/CN  
L2 3602 S MALEIC ACID  
L3 1 S MALEIC ACID/CN  
L4 1 S BUTANEDIOIC ACID/CN  
L5 3 S COPPER OXIDE/CN  
L6 0 S GAMMA-BUTYROLACTONE/CN  
L7 1 S BUTYROLACTONE/CN

FILE 'CAPLUS, CAOLD' ENTERED AT 10:46:40 ON 13 SEP 2006

L8 91 S L1 AND L5  
L9 4 S L8 AND L3  
L10 45 S L8 AND L7  
L11 3 S L10 AND L3  
L12 0 S L11 NOT L9  
L13 1 S L10 AND L4  
L14 1 S L13 NOT L9  
L15 27786 S 1,4-BUTANEDIOL OR ?BUTANE-1,4-DIOL  
L16 100 S L15 AND L5  
L17 0 S L16 AND ?BLACTONE  
L18 51 S L16 AND ?LACTONE  
L19 28 S L18 AND HYDROGENAT?  
L20 19 S L19 AND L7  
L21 17 S L20 NOT L9  
L22 16 S L21 NOT L14  
L23 7 S L22 AND PHASE  
L24 9 S L22 NOT L23

FILE 'CASREACT' ENTERED AT 11:21:44 ON 13 SEP 2006

L25 STRUCTURE UPLOADED  
L26 STRUCTURE UPLOADED  
L27 37 S L25  
L28 840 S L25 FUL  
L29 6 S L26  
L30 132 S L26 FUL  
L31 9 S L28 AND L30  
L32 0 S L31 AND L5  
L33 5 S L27 AND HYDROGENAT?  
L34 0 S L33 AND COPPER  
L35 803 S L28 NOT L27  
L36 112 S L35 AND HYDROGENAT?  
L37 7 S L36 AND COPPER  
L38 33 S L30 AND HYDROGENAT?  
L39 7 S L38 AND COPPER  
L40 7208 S 39 NOT L37  
L41 7 S L39 NOT L37



chain nodes :

6 7 8 9 10 11 12

ring nodes :

1 2 3 4 5

chain bonds :

3-6 7-8 7-12 8-9 9-10 10-11

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5

exact bonds :

7-8 7-12 8-9 9-10 10-11

Match level :

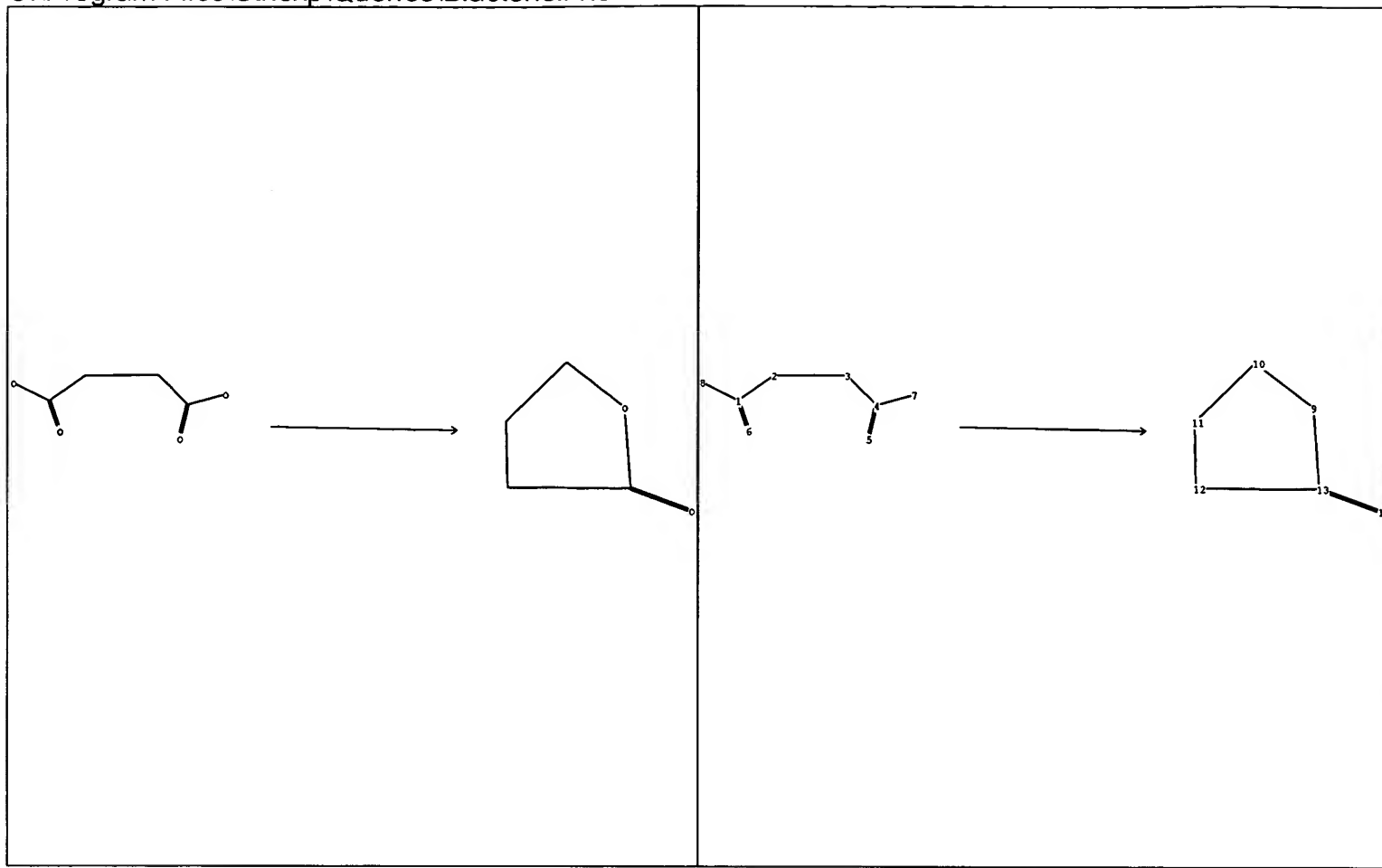
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS  
12:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

containing 1



chain nodes :

1 2 3 4 5 6 7 8 14

ring nodes :

9 10 11 12 13

chain bonds :

1-2 1-6 1-8 2-3 3-4 4-5 4-7 13-14

ring bonds :

9-10 9-13 10-11 11-12 12-13

exact/norm bonds :

1-6 1-8 4-5 4-7 9-10 9-13 10-11 11-12 12-13 13-14

exact bonds :

1-2 2-3 3-4

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:CLASS

fragments assigned product role:

containing 9

fragments assigned reactant/reagent role:

containing 1